

Research Article

Extendability of Equilibria of Nematic Polymers

Hongyun Wang¹ and Hong Zhou²

¹ Department of Applied Mathematics and Statistics, University of California, Santa Cruz, CA 95064, USA

² Department of Applied Mathematics, Naval Postgraduate School, Monterey, CA 93943, USA

Correspondence should be addressed to Hong Zhou, hzhou@nps.edu

Received 9 May 2008; Accepted 30 October 2008

Recommended by Nobuyuki Kenmochi

The purpose of this paper is to study the extendability of equilibrium states of rodlike nematic polymers with the Maier-Saupe intermolecular potential. We formulate equilibrium states as solutions of a nonlinear system and calculate the determinant of the Jacobian matrix of the nonlinear system. It is found that the Jacobian matrix is nonsingular everywhere except at two equilibrium states. These two special equilibrium states correspond to two points in the phase diagram. One point is the folding point where the stable prolate branch folds into the unstable prolate branch; the other point is the intersection point of the nematic branch and the isotropic branch where the unstable prolate state becomes the unstable oblate state. Our result establishes the existence and uniqueness of equilibrium states in the presence of small perturbations away from these two special equilibrium states.

Copyright © 2008 H. Wang and H. Zhou. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

1. Introduction

Liquid crystal polymers (LCPs) consisting of rigid rodlike macromolecules in a viscous solvent have wide technological applications [1–4]. The most common theoretical framework for modeling nematic polymers is to represent the nematogenic molecules as rigid rods and to describe the ensemble with an orientational probability density function (pdf) [5]. Equilibrium orientational distribution is related to the interaction potential by the Boltzmann relation. Recently, rigorous mathematical analysis on the equilibrium states of nematic polymers has garnered serious attention from mathematicians led by Constantin and Titi [6–22]. For example, various proofs for the axisymmetry of equilibrium states with only the Maier-Saupe interaction were given in [8, 19] for the 2-D case and in [9, 18, 20] for the 3-D case; the equilibrium states for the case where dipole-dipole interaction is coupled to the Maier-Saupe interaction were studied in [17, 21]. Not surprisingly, many mathematical issues of polymers are still unexplored. In particular, to our knowledge, the extendability of the equilibrium states has never been attempted.

Report Documentation Page				Form Approved OMB No. 0704-0188	
Public reporting burden for the collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to a penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.					
1. REPORT DATE MAY 2008		2. REPORT TYPE		3. DATES COVERED 00-00-2008 to 00-00-2008	
4. TITLE AND SUBTITLE Extendability of Equilibria of Nematic Polymers				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Naval Postgraduate School, Department of Applied Mathematics, Monterey, CA, 93943				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT Same as Report (SAR)	18. NUMBER OF PAGES 10	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			

In our previous study [21], it was revealed that for large values of the nematic strength and small perturbations, there exists at least one solution near the corresponding unperturbed pure nematic solution. In [21], we concluded the existence using complicated free energy arguments. Moreover, in [21] only existence was established whereas the uniqueness was not addressed at all. Our goal in the current study is to establish rigorously the extendability, both existence and uniqueness, of the equilibrium states of nematic polymers in the presence of small perturbations. Notice that all equilibrium states of nematic polymers are axisymmetric [9, 18, 20]. To facilitate the discussion of extendability, we introduce two new variables for the nonlinear system governing the equilibrium states: one variable is proportional to the order parameter of the pdf; the other variable is proportional to the biaxial order parameter, which measures the deviation of the pdf from being axisymmetric. One advantage of this approach is that the Jacobian matrix is diagonal at equilibrium states. We will show that the Jacobian determinant of the nonlinear system is nonzero everywhere except at two equilibrium states. These two equilibrium states correspond to two points in the phase diagram: one point is the folding point where the stable prolate branch folds into the unstable prolate branch; the other point is the intersection point of the nematic states and the isotropic states where the unstable prolate state becomes the unstable oblate state. The extendability of the equilibrium states except these two states follows immediately from the implicit function theorem.

2. Nonlinear system for equilibrium states, Jacobian matrix, and its determinant

We now briefly recall the mathematical description for equilibrium states of rigid rodlike nematic polymers. The orientation direction of each polymer rod is denoted by a unit vector \mathbf{m} . In this study, by “pure nematic polymers,” we mean the case where the Maier-Saupe interaction potential is the only potential. The Maier-Saupe potential is given by

$$U(\mathbf{m}) = -b\langle \mathbf{m}\mathbf{m} \rangle : \mathbf{m}\mathbf{m}, \quad (2.1)$$

where the tensor product $\mathbf{m}\mathbf{m}$ and the tensor double contraction $\mathbf{A} : \mathbf{B}$ are defined as

$$\mathbf{m}\mathbf{m} \equiv \begin{bmatrix} m_1m_1 & m_1m_2 & m_1m_3 \\ m_2m_1 & m_2m_2 & m_2m_3 \\ m_3m_1 & m_3m_2 & m_3m_3 \end{bmatrix}, \quad (2.2)$$

$$\mathbf{A} : \mathbf{B} \equiv \text{trace}(\mathbf{A}\mathbf{B}).$$

In (2.1), $b = 3N/2$, N is the normalized polymer concentration describing the strength of intermolecular interactions, and $\langle \mathbf{m}\mathbf{m} \rangle$ is the second moment of the orientation distribution:

$$\langle \mathbf{m}\mathbf{m} \rangle \equiv \int_{\|\mathbf{m}\|=1} \mathbf{m}\mathbf{m} \rho(\mathbf{m}) d\mathbf{m}, \quad (2.3)$$

where $\rho(\mathbf{m})$ is the orientational probability density function (pdf) of the ensemble of polymer rods. For convenience, potential (2.1) has been normalized with respect to $k_B T$, where k_B

is the Boltzmann constant and T the absolute temperature. For pure nematic polymers, equilibrium states are described by the Boltzmann distribution [5]:

$$\rho(\mathbf{m}) = \frac{1}{Z} \exp[-U(\mathbf{m})], \quad (2.4)$$

where $Z = \int_S \exp[-U(\mathbf{m})] d\mathbf{m}$ is the partition function and S is the unit sphere.

We choose the coordinate system such that the second moment $\langle \mathbf{m}\mathbf{m} \rangle$ is diagonal:

$$\langle \mathbf{m}\mathbf{m} \rangle = \begin{bmatrix} \langle m_1^2 \rangle & 0 & 0 \\ 0 & \langle m_2^2 \rangle & 0 \\ 0 & 0 & \langle m_3^2 \rangle \end{bmatrix}. \quad (2.5)$$

As a consequence, the Maier-Saupe potential can be written as

$$U(\mathbf{m}) = -b(\langle m_1^2 \rangle m_1^2 + \langle m_2^2 \rangle m_2^2 + \langle m_3^2 \rangle m_3^2). \quad (2.6)$$

The most significant conclusion for pure nematic polymers is that all equilibrium states are axisymmetric [9, 18, 20]. Since not all equilibrium states of a perturbed nematic polymer ensemble are necessarily axisymmetric, to study the extendability, we formulate the problem without using the axisymmetry so that non-axisymmetric perturbations are allowed. The axisymmetry will be useful in our analysis because the extendability is determined by the Jacobian determinant evaluated at the unperturbed equilibrium state, which is axisymmetric. The definition and derivation of the Jacobian matrix, however, require non-axisymmetric formulation. For pure nematic polymers, the total potential is completely specified by the second moment $\langle \mathbf{m}\mathbf{m} \rangle$. As a result of the Boltzmann relation (2.4), an equilibrium state is completely specified by the second moment $\langle \mathbf{m}\mathbf{m} \rangle$. Because of the constraint $m_1^2 + m_2^2 + m_3^2 = 1$, an equilibrium state is completely specified by

$$s_1 \equiv \langle m_1^2 \rangle, \quad s_2 \equiv \langle m_2^2 \rangle. \quad (2.7)$$

At a pure nematic equilibrium state without perturbation, we have $s_1 = s_2$ or $s_1 = 1 - s_1 - s_2$ (which means $s_1 = s_3$) or $s_2 = 1 - s_1 - s_2$ (which means $s_2 = s_3$). At an equilibrium state, we select the coordinate system such that the equilibrium satisfies $s_1 = s_2$. In terms of (s_1, s_2) , the Maier-Saupe potential can be expressed as

$$\begin{aligned} U(\mathbf{m}) &= -b(s_1 m_1^2 + s_2 m_2^2 + (1 - s_1 - s_2) m_3^2) \\ &= -b \left[\frac{1}{2} (s_2 - s_1) (m_2^2 - m_1^2) + \left(1 - \frac{3}{2} (s_1 + s_2) \right) m_3^2 \right] + \text{const.} \end{aligned} \quad (2.8)$$

Consequently, the equilibrium pdf is given by

$$\rho(\mathbf{m}) = \frac{1}{Z} \exp \left\{ b \left[\frac{1}{2} (s_2 - s_1) (m_2^2 - m_1^2) + \left(1 - \frac{3}{2} (s_1 + s_2) \right) m_3^2 \right] \right\}. \quad (2.9)$$

At an equilibrium state, (s_1, s_2) satisfies the nonlinear system:

$$s_1 - \langle m_1^2 \rangle = 0, \quad s_2 - \langle m_2^2 \rangle = 0. \quad (2.10)$$

The form of the equilibrium pdf (2.9) motivates us to introduce (η_1, η_2) :

$$\eta_1 \equiv b \left[1 - \frac{3}{2}(s_1 + s_2) \right], \quad \eta_2 \equiv b \frac{(s_2 - s_1)}{2}. \quad (2.11)$$

Here η_1 is proportional to the order parameter of the pdf while η_2 is proportional to the biaxial order parameter, which measures the deviation of the pdf from being axisymmetric. As we will see, one advantage of using (η_1, η_2) is that the Jacobian matrix is diagonal at equilibrium states. In terms of (η_1, η_2) , the pdf has the expression

$$\rho(\mathbf{m}, \eta_1, \eta_2) = \frac{\exp [\eta_2(m_2^2 - m_1^2) + \eta_1 m_3^2]}{\int_S \exp [\eta_2(m_2^2 - m_1^2) + \eta_1 m_3^2] d\mathbf{m}}. \quad (2.12)$$

The second advantage of using (η_1, η_2) is that the pdf does not depend on b explicitly. Later on, this property will enable us to write b as a function of r which is the equilibrium value of η_1 . At an equilibrium state, the nonlinear system for (η_1, η_2) is

$$\begin{aligned} F_1(\eta_1, \eta_2; b) &\equiv \frac{\eta_1}{b} - \frac{1}{2}(3\langle m_3^2 \rangle - 1) = 0, \\ F_2(\eta_1, \eta_2; b) &\equiv \frac{\eta_2}{b} - \frac{1}{2}\langle m_2^2 - m_1^2 \rangle = 0. \end{aligned} \quad (2.13)$$

In this paper, we study the extendability of equilibrium states of nematic polymers in the presence of small perturbations. We consider a perturbed version of system (2.13):

$$\begin{aligned} F_1(\eta_1, \eta_2; b) &= \epsilon_1, \\ F_2(\eta_1, \eta_2; b) &= \epsilon_2. \end{aligned} \quad (2.14)$$

Mathematically, we study the existence and uniqueness of solution of system (2.14) near a solution of system (2.13) for small ϵ_1 and ϵ_2 . According to the implicit function theorem, the existence and uniqueness are determined by the Jacobian determinant of $(F_1(\eta_1, \eta_2), F_2(\eta_1, \eta_2))$. To calculate the Jacobian matrix, we first calculate the derivatives of pdf (2.12):

$$\begin{aligned} \frac{\partial}{\partial \eta_1} \rho(\mathbf{m}, \eta_1, \eta_2) &= (m_3^2 - \langle m_3^2 \rangle) \rho(\mathbf{m}, \eta_1, \eta_2), \\ \frac{\partial}{\partial \eta_2} \rho(\mathbf{m}, \eta_1, \eta_2) &= (m_2^2 - m_1^2 - \langle m_2^2 - m_1^2 \rangle) \rho(\mathbf{m}, \eta_1, \eta_2). \end{aligned} \quad (2.15)$$

Recall that at a pure nematic equilibrium state without perturbation, we have selected our coordinate system such that $\eta_2 = 0$. Evaluating the partial derivatives of F_1 and F_2 at the equilibrium ($\eta_1 = r, \eta_2 = 0$) yields

$$\begin{aligned}
\left. \frac{\partial}{\partial \eta_1} F_1(\eta_1, \eta_2; b) \right|_{\eta_1=r, \eta_2=0} &= \frac{1}{b} - \frac{3}{2} \langle m_3^2 (m_3^2 - \langle m_3^2 \rangle) \rangle = \frac{1}{b} - \frac{3}{2} \text{var} (m_3^2), \\
\left. \frac{\partial}{\partial \eta_2} F_1(\eta_1, \eta_2; b) \right|_{\eta_1=r, \eta_2=0} &= -\frac{3}{2} \langle m_3^2 (m_2^2 - m_1^2 - \langle m_2^2 - m_1^2 \rangle) \rangle = 0, \\
\left. \frac{\partial}{\partial \eta_1} F_2(\eta_1, \eta_2; b) \right|_{\eta_1=r, \eta_2=0} &= -\frac{1}{2} \langle (m_2^2 - m_1^2) (m_3^2 - \langle m_3^2 \rangle) \rangle = 0, \\
\left. \frac{\partial}{\partial \eta_2} F_2(\eta_1, \eta_2; b) \right|_{\eta_1=r, \eta_2=0} &= \frac{1}{b} - \frac{1}{2} \langle (m_2^2 - m_1^2) (m_2^2 - m_1^2 - \langle m_2^2 - m_1^2 \rangle) \rangle, \\
&= \frac{1}{b} - \frac{1}{2} \langle (m_2^2 - m_1^2)^2 \rangle.
\end{aligned} \tag{2.16}$$

Here we point out that the Jacobian matrix of system (2.13) evaluated at an equilibrium state is diagonal, which is caused by the axisymmetry of the equilibrium state.

It follows that the determinant of Jacobian matrix of system (2.13) at the equilibrium is

$$\det \left(\frac{\partial (F_1, F_2)}{\partial (\eta_1, \eta_2)} \right) \Big|_{\eta_1=r, \eta_2=0} = \left(\frac{1}{b} - \frac{3}{2} \text{var} (m_3^2) \right) \cdot \left(\frac{1}{b} - \frac{1}{2} \langle (m_2^2 - m_1^2)^2 \rangle \right). \tag{2.17}$$

In (2.17), all averages are evaluated using the equilibrium pdf

$$\rho(\mathbf{m}, \eta_1, \eta_2) \Big|_{\eta_1=r, \eta_2=0} = \frac{1}{Z} \exp(r m_3^2). \tag{2.18}$$

For pure nematic polymers, an equilibrium state is completely specified by r . The governing equation for r is the first equation of (2.13): $F_1(r, 0; b) = 0$, whereas the second equation of (2.13) is satisfied automatically when $\eta_2 = 0$. We introduce a new function:

$$F(\eta; b) \equiv F_1(\eta, 0; b) = \frac{\eta}{b} - \frac{1}{2} (3 \langle m_3^2 \rangle - 1). \tag{2.19}$$

The governing equation for r is $F(r; b) = 0$. It follows directly from the definition that function $F(\eta; b)$ is related to the (1, 1) element of the Jacobian matrix at equilibrium as

$$\left. \frac{\partial}{\partial \eta_1} F_1(\eta_1, \eta_2; b) \right|_{\eta_1=r, \eta_2=0} = \left. \frac{\partial}{\partial \eta} F(\eta; b) \right|_{\eta=r}. \tag{2.20}$$

As we will find later, this relation is a key tool for determining the sign of the (1, 1) element of the Jacobian matrix at equilibrium. In the above, we have used variables η and r more or less interchangeably. Later on when necessary, we will use η to denote the independent variable

of functions and use r to denote the particular value of η that satisfies $F(r; b) = 0$. For that purpose, we will continue using these two variables.

3. Extendability of equilibria of nematic polymers

To obtain more specific properties of equilibrium states of nematic polymers, we rewrite the governing equation for r using spherical coordinates. We select the m_3 -axis as the pole of the spherical coordinate system. The equilibrium pdf given in (2.18) becomes

$$\rho(\phi, \theta; r) = \frac{\exp(r \cos^2 \phi)}{2\pi \int_0^\pi \exp(r \cos^2 \phi) \sin \phi d\phi}, \quad (3.1)$$

where ϕ is the polar angle and θ the azimuthal angle. Here we need to point out that r is not the radius in the spherical coordinate system. It is a parameter of the equilibrium state. Substituting equilibrium pdf (3.1) into $(1/2)(3\langle m_3^2 \rangle - 1)$, using a change of variable $u = \cos \phi$, and integrating by parts, we have

$$\frac{1}{2}(3\langle m_3^2 \rangle - 1) = r \cdot \frac{\int_0^1 (u^2 - u^4) \exp(r u^2) du}{\int_0^1 \exp(r u^2) du}. \quad (3.2)$$

Thus, $F(\eta; b)$ defined in (2.19) becomes $F(\eta; b) = \eta[1/b - f(\eta)]$, where $f(\eta)$ is defined as

$$f(\eta) \equiv \frac{\int_0^1 u^2 (1 - u^2) \exp(\eta u^2) du}{\int_0^1 \exp(\eta u^2) du}. \quad (3.3)$$

The equation for r , $F(r; b) = 0$, becomes

$$r \left[\frac{1}{b} - f(r) \right] = 0. \quad (3.4)$$

Equation (3.4) has a trivial solution $r = 0$ for arbitrary value of b , which corresponds to the isotropic branch of the nematic polymer phase diagram. At $r = 0$, the equilibrium pdf is uniform, $\rho(\phi, \theta; 0) = 1/4\pi$. It follows that

$$\begin{aligned} \langle m_j^2 \rangle &= \frac{1}{3}, \\ \langle m_j^4 \rangle &= \langle m_3^4 \rangle = \int_0^1 u^4 du = \frac{1}{5}, \\ \langle m_i^2 m_j^2 \rangle &= \langle m_1^2 m_3^2 \rangle = \frac{1}{2} \int_0^1 u^2 (1 - u^2) du = \frac{1}{15}, \quad i \neq j, \\ \text{var}(m_3^2) &= \langle m_3^4 \rangle - \langle m_3^2 \rangle^2 = \frac{1}{5} - \frac{1}{9} = \frac{4}{45}, \\ \langle (m_2^2 - m_1^2)^2 \rangle &= \langle m_2^4 \rangle - 2\langle m_1^2 m_2^2 \rangle + \langle m_1^4 \rangle = \frac{2}{5} - \frac{2}{15} = \frac{4}{15}. \end{aligned} \quad (3.5)$$

Substituting these results into (2.16), we obtain

$$\begin{aligned}\left.\frac{\partial}{\partial \eta_1} F_1(\eta_1, \eta_2; b)\right|_{\eta_1=0, \eta_2=0} &= \frac{1}{b} - \frac{3}{2} \text{var}(m_3^2) = \frac{1}{b} - \frac{2}{15}, \\ \left.\frac{\partial}{\partial \eta_2} F_2(\eta_1, \eta_2; b)\right|_{\eta_1=0, \eta_2=0} &= \frac{1}{b} - \frac{1}{2} \langle (m_2^2 - m_1^2)^2 \rangle = \frac{1}{b} - \frac{2}{15}.\end{aligned}\quad (3.6)$$

Therefore, when $b \neq 15/2$, the Jacobian matrix is nonsingular and thereby the isotropic equilibrium is extendable. At $b = 15/2$, the isotropic branch intersects with the nematic branch.

The remaining solutions of (3.4), if any, satisfy

$$\frac{1}{b} - f(r) = 0. \quad (3.7)$$

In [20], it has been shown that the function $f(\eta)$ has the following properties:

- (1) $f(0) = 2/15$, $\lim_{\eta \rightarrow +\infty} f(\eta) = 0$ and $\lim_{\eta \rightarrow -\infty} f(\eta) = 0$;
- (2) $f(\eta)$ attains its maximum at $\eta = \eta^* = 2.1782879748 > 0$, where the maximum is $f(\eta^*) = 0.14855559992254 > 0$;
- (3) $f'(\eta) > 0$ for $\eta < \eta^*$ and $f'(\eta) < 0$ for $\eta > \eta^*$.

A graph of $f(\eta)$ is shown in Figure 1(a). Thus, we draw conclusions below for (3.7) as follows.

- (i) The critical value of b is $b^* = 1/f(\eta^*) = 6.7314863965$.
- (ii) For $b < b^*$, (3.7) has no solution.
- (iii) At $b = b^*$, (3.7) has one solution $r(b^*) = \eta^* > 0$.
- (iv) For $b^* < b < 2/15$, (3.7) has two solutions: $r_U(b) > \eta^* > 0$ and $0 < r_M(b) < \eta^*$.
- (v) At $b = 2/15$, (3.7) has two solutions: $r_U(2/15) > \eta^* > 0$ and $r(2/15) = 0$.
- (vi) For $b > 2/15$, (3.7) has two solutions: $r_U(b) > \eta^* > 0$ and $r_L(b) < 0$.

As mentioned before, we use subscript “U” to denote to the “Upper” part of the phase diagram where $r > \eta^*$, subscript “M” to denote to the “Middle” part of the phase diagram, where $0 < r < \eta^*$, and subscript “L” to denote to the “Lower” part of the phase diagram, where $r < 0$. The phase diagram for nematic polymers is shown in Figure 1(b). In the terminologies of nematic polymers, curve segment $r_U(b)$ is the stable part of the prolate branch; $r_M(b)$ is the unstable part of the prolate branch; and $r_L(b)$ is the unstable oblate branch.

Recall that b is the strength of the Maier-Saupe interaction, which is proportional to the normalized polymer concentration and is inversely proportional to the temperature. r , the solution of $F(r; b) = 0$, has the expression $r = b \cdot (1/2)(3\langle m_3^2 \rangle - 1)$, where $(1/2)(3\langle m_3^2 \rangle - 1)$ is the order parameter. Thus, from physical considerations, it is desirable to use b as the independent variable and treat r as a function of b . However, $r(b)$ is a multivalued function of b and for $b < b^*$ function $r(b)$ is not even defined. Mathematically, it is much more convenient if we use r as the independent variable and treat b as a function of r . $b(r)$ is a

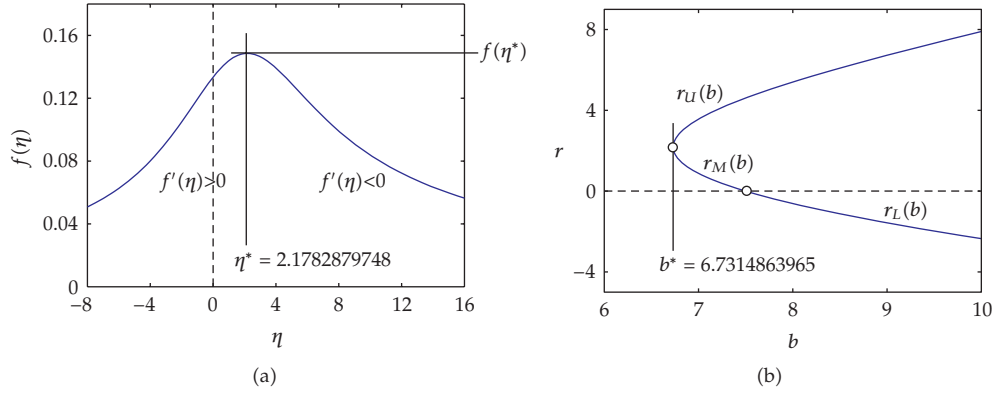


Figure 1: (a) Graph of function $f(\eta)$; (b) phase diagram of nematic polymers.

single-value function of r and is defined for all values of r in $(-\infty, +\infty)$. Below, we will adopt this new formulation of viewing b as a function of r . In the new formulation, function $b(r)$ is determined from (3.7) as $b(r) = 1/f(r)$. In terms of this new formulation, the stable part of the prolate branch $r_U(b)$ can be simply represented as $b(r)$ for $r > \eta^*$; the unstable part of the prolate branch $r_M(b)$ as $b(r)$ for $0 < r < \eta^*$; and the unstable oblate branch $r_L(b)$ as $b(r)$ for $r < 0$. Now we discuss the extendability of these branches. Using relation (2.20), $F(\eta; b) = \eta[1/b - f(\eta)]$, and $1/b - f(r) = 0$, we arrive at

$$\begin{aligned}
 \left. \frac{\partial}{\partial \eta_1} F_1(\eta_1, \eta_2; b(r)) \right|_{\eta_1=r, \eta_2=0} &= \left. \frac{\partial}{\partial \eta} F(\eta; b(r)) \right|_{\eta=r} \\
 &= \left[\frac{1}{b(r)} - f(\eta) \right] \bigg|_{\eta=r} - \eta f'(\eta) \bigg|_{\eta=r} \\
 &= -r f'(r) = \begin{cases} > 0, & \text{for } r > \eta^* \\ < 0, & \text{for } 0 < r < \eta^* \\ > 0, & \text{for } r < 0. \end{cases}
 \end{aligned} \tag{3.8}$$

To study the (2,2) element of Jacobian matrix, we first rewrite $(1/2)\langle (m_2^2 - m_1^2)^2 \rangle$ by substituting equilibrium pdf (3.1) into $(1/2)\langle (m_2^2 - m_1^2)^2 \rangle$ and using substitution $u = \cos \phi$,

$$\frac{1}{2} \langle (m_2^2 - m_1^2)^2 \rangle = \frac{1}{4} \frac{\int_0^1 (1-u^2)^2 \exp(ru^2) du}{\int_0^1 \exp(ru^2) du}. \tag{3.9}$$

Using (2.16), $b(1) = 1/f(r)$, the expression of $f(r)$ given in (3.3), and result (3.9), we have

$$\begin{aligned}
 \left. \frac{\partial}{\partial \eta_2} F_2(\eta_1, \eta_2; b(r)) \right|_{\eta_1=r, \eta_2=0} &= \frac{1}{b(r)} - \frac{1}{2} \langle (m_2^2 - m_1^2)^2 \rangle \\
 &= \frac{1}{4} \frac{\int_0^1 (1-u^2)(5u^2-1) \exp(ru^2) du}{\int_0^1 \exp(ru^2) du} \equiv g(r).
 \end{aligned} \tag{3.10}$$

It is straightforward to verify that $g(0) = 0$. Below, we want to show that $g(r) > 0$ for $r > 0$ and $g(r) < 0$ for $r < 0$. To facilitate the analysis below, we write $g(r)$ as an average

$$g(r) = \frac{1}{4} \langle (1 - u^2)(5u^2 - 1) \rangle, \quad (3.11)$$

where the average is with respect to the pdf $\rho(u; r) = \exp(ru^2) / \int_0^1 \exp(ru^2) du$.

Lemma 3.1. *Function $g(r)$ given in (3.11) has the property that $g(r) = 0$ implies $g'(r) > 0$.*

Proof of Lemma 3.1. We first calculate the derivative of the pdf: $(\partial/\partial r)\rho(u; r) = (u^2 - \langle u^2 \rangle)\rho(u; r)$, which leads to

$$\begin{aligned} g'(r) &= \frac{1}{4} \langle (1 - u^2)(5u^2 - 1)(u^2 - \langle u^2 \rangle) \rangle \\ &= \frac{1}{20} \langle (1 - u^2)(5u^2 - 1)^2 \rangle + \frac{1}{5} (1 - 5\langle u^2 \rangle) g(r). \end{aligned} \quad (3.12)$$

Thus, whenever $g(r) = 0$, we have $g'(r) = (1/20) \langle (1 - u^2)(5u^2 - 1)^2 \rangle > 0$. \square

Lemma 3.1 together with $g(0) = 0$ leads to $g(r) > 0$ for $r > 0$ and $g(r) < 0$ for $r < 0$. Combining this result on $g(r)$ with result (3.8) on $-rf'(r)$, we arrive at

$$\det \left(\frac{\partial(F_1, F_2)}{\partial(\eta_1, \eta_2)} \right) \Big|_{\eta_1=r, \eta_2=0} = (-rf'(r))g(r) = \begin{cases} > 0, & \text{for } r > \eta^*, \\ < 0, & \text{for } 0 < r < \eta^*, \\ < 0, & \text{for } r < 0. \end{cases} \quad (3.13)$$

Therefore, we conclude that all nematic equilibrium states (stable or unstable) are extendable except for the equilibrium state at $(r = 0, b = 15/2)$ and the equilibrium state at $(r = \eta^*, b = b^*)$.

4. Conclusions

In this work, we studied the extendability of equilibrium states of nematic polymers with the Maier-Saupe intermolecular potential. We found that the Jacobian matrix of the nonlinear system is nonsingular except at two special equilibrium states. The significance of this result is its implication on the existence and uniqueness of equilibrium states of a perturbed system, in the neighborhood of the unperturbed equilibrium states.

Acknowledgments

H. Wang was partially supported by the National Science Foundation. H. Zhou was supported in part by the Air Force Office of Scientific Research under Grant no. F1ATA06313G003.

References

- [1] B. Bird, R. C. Armstrong, and O. Hassager, *Dynamics of Polymeric Liquids*, vol. 1, John Wiley & Sons, New York, NY, USA, 1987.
- [2] A. M. Donald, A. H. Windle, and S. Hanna, *Liquid Crystalline Polymers*, Cambridge University Press, Cambridge, UK, 2nd edition, 2006.
- [3] S. Hess and M. Kröger, "Regular and chaotic orientational and rheological behaviour of liquid crystals," *Journal of Physics: Condensed Matter*, vol. 16, no. 38, pp. S3835–S3859, 2004.
- [4] A. D. Rey and M. M. Denn, "Dynamical phenomena in liquid-crystalline materials," in *Annual Review of Fluid Mechanics*, vol. 34 of *Annual Review of Fluid Mechanics*, pp. 233–266, Annual Reviews, Palo Alto, Calif, USA, 2002.
- [5] M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics*, Oxford University Press, Oxford, UK, 1986.
- [6] P. Constantin, I. G. Kevrekidis, and E. S. Titi, "Asymptotic states of a Smoluchowski equation," *Archive for Rational Mechanics and Analysis*, vol. 174, no. 3, pp. 365–384, 2004.
- [7] P. Constantin, I. Kevrekidis, and E. S. Titi, "Remarks on a Smoluchowski equation," *Discrete and Continuous Dynamical Systems. Series A*, vol. 11, no. 1, pp. 101–112, 2004.
- [8] P. Constantin and J. Vukadinovic, "Note on the number of steady states for a two-dimensional Smoluchowski equation," *Nonlinearity*, vol. 18, no. 1, pp. 441–443, 2005.
- [9] I. Fatkullin and V. Slastikov, "Critical points of the Onsager functional on a sphere," *Nonlinearity*, vol. 18, no. 6, pp. 2565–2580, 2005.
- [10] M. G. Forest, R. Zhou, and Q. Wang, "Symmetries of the Doi kinetic theory for nematic polymers of arbitrary aspect ratio: at rest and in linear flows," *Physical Review E*, vol. 66, no. 3, Article ID 031712, 9 pages, 2002.
- [11] M. G. Forest, Q. Wang, and R. Zhou, "The flow-phase diagram of Doi-Hess theory for sheared nematic polymers II: finite shear rates," *Rheologica Acta*, vol. 44, no. 1, pp. 80–93, 2004.
- [12] M. G. Forest, Q. Wang, and R. Zhou, "The weak shear kinetic phase diagram for nematic polymers," *Rheologica Acta*, vol. 43, no. 1, pp. 17–37, 2004.
- [13] M. G. Forest, R. Zhou, and Q. Wang, "Chaotic boundaries of nematic polymers in mixed shear and extensional flows," *Physical Review Letters*, vol. 93, no. 8, Article ID 088301, 4 pages, 2004.
- [14] R. Zhou, M. G. Forest, and Q. Wang, "Kinetic structure simulations of nematic polymers in plane Couette cells—I: the algorithm and benchmarks," *Multiscale Modeling & Simulation*, vol. 3, no. 4, pp. 853–870, 2005.
- [15] M. G. Forest, R. Zhou, and Q. Wang, "Scaling behavior of kinetic orientational distributions for dilute nematic polymers in weak shear," *Journal of Non-Newtonian Fluid Mechanics*, vol. 116, no. 2-3, pp. 183–204, 2004.
- [16] M. G. Forest and Q. Wang, "Monodomain response of finite-aspect-ratio macromolecules in shear and related linear flows," *Rheologica Acta*, vol. 42, no. 1-2, pp. 20–46, 2003.
- [17] G. Ji, Q. Wang, P. Zhang, and H. Zhou, "Study of phase transition in homogeneous, rigid extended nematics and magnetic suspensions using an order-reduction method," *Physics of Fluids*, vol. 18, no. 12, Article ID 123103, 17 pages, 2006.
- [18] H. Liu, H. Zhang, and P. Zhang, "Axial symmetry and classification of stationary solutions of Doi-Onsager equation on the sphere with Maier-Saupe potential," *Communications in Mathematical Sciences*, vol. 3, no. 2, pp. 201–218, 2005.
- [19] C. Luo, H. Zhang, and P. Zhang, "The structure of equilibrium solutions of the one-dimensional Doi equation," *Nonlinearity*, vol. 18, no. 1, pp. 379–389, 2005.
- [20] H. Zhou, H. Wang, M. G. Forest, and Q. Wang, "A new proof on axisymmetric equilibria of a three-dimensional Smoluchowski equation," *Nonlinearity*, vol. 18, no. 6, pp. 2815–2825, 2005.
- [21] H. Zhou, H. Wang, Q. Wang, and M. G. Forest, "Characterization of stable kinetic equilibria of rigid, dipolar rod ensembles for coupled dipole-dipole and Maier-Saupe potentials," *Nonlinearity*, vol. 20, no. 2, pp. 277–297, 2007.
- [22] H. Zhou, H. Wang, and Q. Wang, "Nonparallel solutions of extended nematic polymers under an external field," *Discrete and Continuous Dynamical Systems. Series B*, vol. 7, no. 4, pp. 907–929, 2007.